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TITLE   GENERAL MANY-BODY SYSTEMS

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INTRODUCTION

The problem of how to visualize and sometimes solve a general many-body system is considered. The ideas are established in the context of very simple small systems, a Hubbard model and a coupled electron-phonon model, both on two lattice sites. These models are also solved to good approximation in the thermodynamic limit, although the Hubbard model is restricted to a small number of holes away from the Mott insulating state. Response functions are also considered.

A fairly general many-body Hamiltonian is

$$H = H_{t,el} + H_{el-el} + H_{el-ph} + H_{ph} . \tag{1}$$

consisting of an electron or other fermion kinetic energy and electron-electron interactions, which may be coupled to a bose field such as a phonon. The phonons themselves may be nonlinear (have self-interactions). The system may be strongly coupled (H_{el-el} and H_{el-ph} may be large). One may also add coupling to an external driving field, such as an AC electric field. The methods discussed are nonperturbative, and so differ from the standard methods of diagrammatic perturbation theory.[1] A comparison is made with diagrammatic methods in the context of the random phase approximation.

HUBBARD MODEL (SMALL SYSTEM)

The first example is the Hubbard model, which describes interacting electrons and contains only the first two terms of Eq. (1):

$$H_{II} = -t \sum_{<j,k>,s} (c'_{j,s} c_{k,s} + h.c.) + U \sum_{j} c_{j\uparrow}^{\dagger} c_{j\uparrow} c_{j\downarrow}^{\dagger} c_{j\downarrow} . \tag{2}$$

The operator $c_{j,s}^{\dagger}$ creates an electron of spin s on a Wannier orbital on lattice site j. The first term (electron kinetic energy) causes electrons to hop to nearest neighbor sites without changing their spin. The last term is a repulsive on site electron-electron interaction. To illustrate the exact solution of Eq. (2) for a small system, consider the problem with two sites, two electrons, and the z-component of the spin S_z, which is conserved, equal to zero. (Infinite systems will be considered later.)

The Hilbert space in coordinate representation is given by

$$
\begin{aligned}
|1> &= \uparrow \qquad \downarrow \\
|2> &= \uparrow\downarrow \\
|3> &= \qquad\quad \uparrow\downarrow \\
|4> &= \downarrow \qquad \uparrow .
\end{aligned}
\tag{3}
$$

where the first site is on the left and the second on the right. The Hamiltonian operating on $|1>$ connects (has nonzero matrix elements) to states $|2>$ and $|3>$. State $|4>$ also connects to $|2>$ and $3>$, see Fig. (1). The diagonal energy of states $|2>$ and $|3>$ is U, and that of $|1>$ and $|4>$ is 0.

Note that an interacting many-body problem (containing the product of four fermion operators) has been mapped onto a non-interacting one particle tight-binding problem. If the operator $b_j^{\dagger}$ creates many-body state $|j>$ in Eq. (3), the new Hamiltonian is

$$\tilde{H} = \sum_{j,k} \tilde{t}_{jk} \, (b_j^+ b_k + h.c.) + \sum_j \tilde{\varepsilon}_j \, b_j^+ b_j \; . \tag{4}$$

with no interactions (four-fermion operators). The sites in the tight-binding problem, however, represent many-body states, not the usual atomic or Wannier orbitals. It is a general result that one can always exactly map the ground and excited states of an interacting many-body problem onto those of a noninteracting one-body problem in this way.

In matrix notation, $\tilde{H}$ is

$$\tilde{H} = \begin{bmatrix} 0 & -t & -t & 0 \\ -t & U & 0 & -t \\ -t & 0 & U & -t \\ 0 & -t & -t & 0 \end{bmatrix} \tag{5}$$

This matrix is simple to diagonalize exactly. The four eigenvalues are

$$(E_1, E_2, E_3, E_4) = ((U - \sqrt{U^2 + 16t^2})/2 \, , \, 0 \, , \, U \, , \, (U + \sqrt{U^2 + 16t^2})/2)$$

The two lowest energy (unnormalized) eigenvectors are

$$|\psi_1> = |1> + |4> + a\,(|2> + |3>)$$

$$|\psi_2> = |1> - |4> \, .$$

where $a = -E_1/2t$. $|\psi_1>$ is a singlet state and $|\psi_2>$ is the $S_z = 0$ triplet state. For $U \gg t$, the low energy part of the Hilbert space is described by

$$H = const + J \, \vec{\sigma}_1 \cdot \vec{\sigma}_2 \, ,$$

with $J = t^2/U$.

It appears that the singlet and triplet states are written with incorrect signs. The signs are in fact correct, which brings up an issue that was glossed over: the ordering of anticommuting fermion operators. For the problem above, the reference ordering is to have the up spins operate first.

$$c_{2\downarrow}^\dagger \, c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger \, c_{1\uparrow}^\dagger \, |0\rangle \,, \tag{6}$$

where $|0\rangle$ is the vacuum. A state with a positive sign is given by operators in the above order, for example $|2\rangle = c_{1\downarrow}^\dagger \, c_{1\uparrow}^\dagger \, |0\rangle$. Suppose one had chosen a different ordering convention, such as putting site 1 operators first:

$$c_{2\downarrow}^\dagger \, c_{2\uparrow}^\dagger \, c_{1\downarrow}^\dagger \, c_{1\uparrow}^\dagger \, |0\rangle \,. \tag{7}$$

The new tight binding model is shown in Fig. (2). The 2-4 bond sign, for example, is obtained with the convention of Eq. (7) as follows:

$$H_t \, |2\rangle = -t \, (c_{2\uparrow}^\dagger c_{1\uparrow}) \, c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger \, |0\rangle = +t \, c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger \, |0\rangle = +t \, |4\rangle \,.$$

The eigenvalues of the new problem (Fig. 2) are the same as those of Fig. 1, and the wavefunctions are "covariant": $(\psi_1, \psi_2, \psi_3, \psi_4)_1 \to (\psi_1, \psi_2, \psi_3, -\psi_4)_2$. Now a singlet is written in the conventional way.

This is in fact a type of gauge transformation. An example of a general tight-binding model is given in Figure (3). If one changes the definition of a basis state (e.g. $|\phi_1\rangle \to -|\phi_1\rangle$), all of the bonds coming from $|\phi_1\rangle$ change sign, as shown in Figure (4). In general any loop with an even number of $+t$ bonds may be transformed into a loop with no $+t$ bonds by a suitable choice of gauge (sign of basis functions). All $+t$ bonds may also be removed from bonds that are not part of a loop, such as 8-9. However, loops with an odd number of $+t$ bonds are frustrated (the $+t$ bonds may not be gauged away). The gauge transformation generalizes to $|\phi_1\rangle \to e^{i\theta}|\phi_1\rangle$, where θ was taken equal to π above.

Similar issues arise in the quantum Hall effect when a magnetic field penetrates a lattice. In that case a flux through a loop that is an integer times the flux quantum ϕ_0 is the same as zero flux under a gauge transformation.

One can write down an approximate ground state of an unfrustrated tight binding model almost by inspection. First gauge transform away all $+t$ bonds. Then all the ψ_j have the same sign in the groundstate, with ψ_j larger on sites that have a lower energy, and more or larger connected t_{ij} bonds.

One can do larger Hubbard models exactly. For example, with 2N sites and 2N electrons, half of which are spin up, one must diagonalize a matrix of size $\left[\dfrac{2N}{N} \right]^2$ on a side. Six sites yield a 400 x 400 matrix, or equivalently a tight-binding model with 400 sites, which can be diagonalized completely on a computer. Ten sites yield a 63,504 x 63,504 matrix, which can be solved for the ground and low lying excited states by the Lanczos method.[2] There is no exact solution for the infinite Hubbard model.

POLARONS (SMALL SYSTEM)

The second example is a coupled electron-phonon system, described by

$$
H = -t \sum_{<j,k>_s} (c_{j,s}^{\dagger} c_{k,s} + h\,c\,) + U \sum_j n_{j\uparrow} n_{j\downarrow} + V \sum_{<j,k>} n_j\, n_k \tag{8}
$$
$$
+ \lambda \sum_j (n_{j\uparrow} + n_{j\downarrow})(a_j + a_j') + \Omega \sum_j a_j^{\dagger} a_j \,.
$$

where $n_{j\uparrow} = c_{j\uparrow}^{\dagger} c_{j\uparrow}$ and $n_j = n_{j\uparrow} + n_{j\downarrow}$. In the 1-d version, electrons run along a chain, possibly interacting with each other on site and on nearest neighbor sites (U and V terms respectively). Each site is coupled to a harmonic oscillator, so that the oscillator feels an extra force when an electron is on that site, $\delta H = -\lambda_1 x$, where x is the phonon coordinate. In terms of the creation operator a' for the oscillator,

$$
\mathscr{C} = \sqrt{\frac{\hbar}{2m\omega}} \, (a + a')\,.
$$

The last term is the energy of the oscillators, with $\Omega = \hbar\omega$ and the zero point energy subtracted

off. This model is for a phonon energy that is independent of $\vec{k}$, or optical phonons. (If $a_j^+ a_k$ terms were added to the Hamiltonian, the phonon energy would have a nonzero dispersion.) The Hamiltonian in Eq. (8) describes the system shown in Figure (5).

For simplicity, consider first a two site problem with 1 electron and two phonons. With only one electron present, the U and V terms do not operate. The basis functions can be taken either in position or momentum space. For variety, and to compare with the random phase approximation (RPA), the calculation will be done in momentum space. For a two site lattice, only $\vec{k} = 0, \pi$ are allowed.

There are 2 electron basis states,

$$|0_{el}\rangle = \frac{1}{\sqrt{2}}(|1_{el}\rangle + |2_{el}\rangle)$$

$$|\pi_{el}\rangle = \frac{1}{\sqrt{2}}(|1_{el}\rangle - |2_{el}\rangle)$$

The energy of the first is $-t$ and of the second is $+t$. There are also two phonon creation operators

$$a_0^+ = \frac{1}{\sqrt{2}}(a_1^+ + a_2^+)$$

$$a_\pi^+ = \frac{1}{\sqrt{2}}(a_1^+ - a_2^+)$$

Each a^+ can create arbitrarily many quanta. A many-body state is specified by

$$|q_{el}\rangle |n_0\rangle |n_\pi\rangle ,$$

where $q_{el} = 0$ or π, and the phonon occupation numbers are $n_0 = 0,1,2,...,$ $n_\pi = 0,1,2,...$. The electron phonon interaction conserves momentum. Its strength is momentum independent in this model.

The equivalent 1-body tight binding model consists of two disconnected pieces for this model, one for each total momentum. The total momentum $K = \pi$ piece of the Hilbert space is shown in Figure (6). The q_{el} can be deduced from the total K, $q = (K - \pi n_\pi) \bmod 2\pi$, so by specifying the phonon state, one also specifies the electron state. The lowest row of vertices has $q_{el} = \pi$, etc.

The diagonal energy of a site is

$$E(n_0, n_\pi) = \Omega(n_0 + n_\pi) + (-1)^{n_\pi} \qquad (K = \pi) .$$

The numerical factors in the off-diagonal matrix elements can be obtained using $a^{\dagger} |n> = \sqrt{n+1} |n+1>$. The energy in Fig. (6) therefore increases linearly to the upper right, with a corrugation as a function of y. In this basis, t appears in a diagonal (site) energy, in contrast to the real-space basis in the previous example, where t is an off-diagonal bond strength. There is an identical lattice for the $K = 0$ sector, except that the y corrugations are opposite,

$$E(n_0, n_\pi) = \Omega(n_0 + n_\pi) - (-1)^{n_\pi} \qquad (K = 0) .$$

To find the ground state and low lying excited states numerically, one truncates the lattice (keeping states to the lower left, with low diagonal energies). The remaining problem is solved numerically. One should check that the truncation does not effect the physics, by verifying that the wavefunctions and energies of the low lying eigenstates have converged.

The interaction with the phonons is said to be retarded or frequency- dependent. In this formulation, however, one need not include an explicitly frequency-dependent interaction, but merely couple in phonon states of various energies on an equal footing with all other states.

How do standard diagrammatic methods, such as the random phase approximation (RPA), compare with solving the equivalent tight-binding lattice? Consider the question of how the $k = \pi$ phonon energy is changed by the electron-phonon interaction. If λ were zero, the bare $k = \pi$

phonon would be an eigenstate of energy $-t + \Omega$. This is the state $(n_0, n_\pi) = (0,1)$ in Fig. (6). The RPA sums all diagrams of the form shown in Figure (7), with any number of bubbles. The vertical line on the left cuts through the state with one $k = \pi$ phonon and no electron-hole pairs, which is state (0,1) in Fig. (6). The vertical line on the right cuts through the state with an electron-hole pair and no phonons, which is the state (0,0). In the exact problem, there are also matrix elements from state (0,1) to (0,2) and to (1,1). These matrix elements are the vertices shown in Figure (8), which are neglected by the RPA.

The RPA thus keeps only the two states (0,1) and (0,0) and the bond between them, and throws away the rest of the lattice, as shown in Figure (9). It solves this tiny ''two site'' problem exactly. When is this a good approximation? One requires $\lambda \ll t$ for there to be no significant admixtures of the neglected state (0,2) in the ground state. Furthermore, $\lambda \ll \Omega$ is required to prevent significant admixtures of state (1,1), which was also neglected. In this limit however, the bare phonon state (0,1) is essentially exact, so that one need not have bothered with more than one state. The RPA is thus not very useful for this case.

Various response functions (Green's functions) can be calculated directly from the eigenstates. For example the optical absorption is

$$\alpha(\omega) = \frac{1}{\omega} \sum_n |\langle n | \hat{j} | 0 \rangle|^2 \, \delta(\omega - (\epsilon_n - \epsilon_0)). \tag{9}$$

where $\hat{j}$ is the current operator. If the Hilbert space is truncated, $\alpha(\omega)$ becomes unreliable for very large ω.

LARGE SYSTEMS

A general large many-body problem cannot be solved by any method, including this one. Consider the Hubbard model with 10^{23} sites at arbitrary filling in the momentum space basis. In

this treatment, the first state (noninteracting fermi ground state) connects via U to an enormous number of states $O(10^{64})$. The problem at this level, which is a very large "star" tight binding model (Fig. 10a), is still straightforward to solve exactly. However, there is no justification for stopping at this level. Each perimeter state connects to a large number of other states, sometimes forming loops, and each of them connects to many new states, etc., so the problem finally becomes intractable. This is illustrated schematically in Fig. (10b). The many-body problem has still been mapped exactly onto a one-body tight-binding problem, but one that is too large to solve.

There is, however, a class of problems that can be solved essentially exactly or to good approximation on an *infinite* lattice. These problems describe the quantum dynamics of one or several "defects" in a well-understood background. Two examples are: (1) The problem in which a small number of electrons interact with optical phonons to form polarons, bipolarons, etc. on an infinite lattice. (2) The problem of holes and pairs of holes in the Mott insulating state of the Hubbard model on an infinite lattice in two or more dimensions.

The polaron problem is the same electron-optical phonon problem described above, but done on an infinite lattice in real space rather than k-space. The many-body basis states are

$$|j> \ |n_j> \ |n_{j+1}> \ |n_{j-1}> \ |n_{j+2}> \ |n_{j-2}> \ ....$$

The first ket is the electron location, followed by the number of phonons on the same site, on nearest neighbor sites, etc. Again one constructs an arbitrarily large variational space, and then checks that the space is big enough.

A small variational space might allow for zero or one phonon on the site that the electron is on or on a nearest neighbor site. (A much larger space is used for accurate calculations.) The small variational space can be written

state	-1	0	1		(10)
1	0	0	0		
2	0	1	0		
3	0	0	1		
4	1	0	0		
5	0	1	1		
6	1	1	0		
7	1	0	1		
8	1	1	1		

The headings show the number of phonons on the site to the left of the electron (-1), on the same site as the electron (0), and to the right of the electron (1). All translations of thes: states are also included in the Hilbert space. The tight-binding lattice is shown in Fig. (11). The vertical bonds have strength $-\lambda$, and the others strength $-t$. The diagonal energy is zero for state 1, Ω for states 2, 3, and 4, and 2Ω for states 5 and 6. Different states with the same number represent translations of a state. For example, the leftmost state 3 represents the state with an electron on site 0 and a phonon on site 1. The middle state 3 represents the state with an electron on site 1 and a phonon on site 2. States 7 and 8 form a disconnected part of the Hilbert space and are not shown. There are $6N$ states in the Hilbert space, where the number of sites N is infinite. The Hilbert space is translation invariant, with 6 states per unit cell. The translation invariance implies that the exact eigenstates obey Bloch's theorem. For any crystal momentum $\vec{k}$, one need diagonalize only a 6×6 hermitian matrix, rather than a $6N \times 6N$ matrix.

The ground state eigenfunction of the tight-binding model describes a polaron. Note that even with this small Hilbert space, there is already more than one way to propagate through the lattice, either directly along the baseline or through a high loop. The loop route shows that the polaron can move by making a virtual internal excitation, and then getting rid of it. Different propagation routes interfere constructively in the physical polaron. The polaron is never "self trapped," but rather is delocalized in a Bloch state of wavevector $\vec{k}$, possibly with a large effective mass.

Plotting the tight-binding eigenvalues as a function of $\vec{k}$ gives a graph that looks like a band structure, although it describes many-body physics. The lowest band is the polaron quasiparticle energy $\varepsilon(\vec{k})$ for the electron dressed with phonons. The higher bands are either excited states of the quasiparticle or unbound electron-phonon states. One can examine how the quasiparticle energy, wavefunction, and residue Z vary with k. Figure (12) shows these bands for a larger variational Hilbert space that includes 100 variational states per lattice site. Other calculations with several thousand variational states, involving many phonons in a large neighborhood of the electron, have been performed. Calculations have also been done for bipolarons, nonlinear phonons, and for the AC conductivity of a polaron.[3]

The same method can be applied to other many-body problems on an infinite lattice. The Hubbard model in two dimensions, with one electron per site forms a Mott insulating state with antiferromagnetic long-range order.[4] The problem of one and two holes in the Mott insulating state and the interaction between the hole has been studied.[5] In this case the variational space consists of the location of the hole(s), and a number of spin-flips relative to the Neel state in the vicinity of the holes. The Green's function for hole propagation, which contains excited state information, has also been obtained.[6] These studies have used a variational space as large as 609 states per real space lattice site.

SUMMARY

For a small system, one can solve essentially exactly for the low-lying eigenvalues, eigenfunctions, and linear response to an external probe. These systems may include electron-electron, electron-phonon, and nonlinear phonon interactions. Standard diagrammatic techniques, like the RPA may be inadequate for these problems. Some infinite systems can be solved exactly or to good approximation by the same technique, which exactly maps a many-body problem onto

a one-body tight-binding model.

References

(1)   See, e.g., A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Pergamon, Elmsford, NY, 1965), S. Doniach and E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin, Reading, MA, 1974), A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, NY, 1971), G. D. Mahan, *Many-Particle Physics* (Plenum, NY, 1981).

(2)   S. Pissanetzky, *Sparse Matrix Technology* (Academic, NY, 1984).

(3)   I. Batistic, S. Marianer, and S. Trugman, unpublished.

(4)   J. D. Reger and A. P. Young, Phys Rev. B 37, 5978 (1988).

(5)   S. A. Trugman, Phys Rev. B 37, 1597 (1988).

(6)   S. A. Trugman, LANL preprint 89 2230.

Figure Captions

Figure 1   The tight-binding model represents the two-site Hubbard model with two electrons, S, 0. The bonds are off diagonal matrix elements of amplitude t.

Figure 2   The modified tight-binding model for the two-site Hubbard model, using the ordering convention in Eq. (7). The slashed bonds are off-diagonal matrix elements of amplitude $+t$, and the unslashed bonds of amplitude $-t$.

Figure 3   A general tight-binding model may contain loops, dead ends, and sites with different coordination numbers.

Figure 4   A gauge transformation of the previous tight-binding model accomplished by $|\phi_1\rangle \rightarrow -|\phi_1\rangle$. The slashed bonds are matrix elements $+t$.

Figure 5   A polaron system in which electrons hop along a chain. Each site on the chain is associated with a harmonic oscillator. If an electron, represented by an arrow, is present on a site, an additional force is applied to the oscillator on that site.

Figure 6   A portion of the infinite tight-binding model representing a coupled electron-phonon system. The sector pictured has total momentum $K = \pi$. A state (site) is labeled by (n_0, n_π), where n_0 is the number of momentum zero phonons and n_π is the number of momentum π phonons. The electron momentum q is shown on the right for each row. The bonds are off-diagonal matrix elements of amplitude λ times a numerical constant.

Figure 7   A diagram retained in the RPA approximation.

Figure 8   Some vertices that are neglected in the RPA approximation. T. · matrix element connecting state (0,1) to state (0,2) is shown diagramatically above, and the one connecting (0,1) to (1,1) is shown below.

Figure 9   For this problem, the RPA retains only the bond and two sites that are shown in black, discarding the rest of the infinite lattice.

Figure 10   (a) The large ''star'' obtained as the first approximation to the Hubbard model in the thermodynamic limit. The off-diagonal matrix elements are allowed to operate only once (b) If the off-diagonal matrix elements are allowed to act repeatedly, each of the sites at the edge connect to many other sites, and each of those connect to many others, etc., sometimes forming

loops. (Shown schematically.)

Figure 11   The tight-binding model for a polaron on an infinite lattice. With the small basis set of Eq. (10), the tight-binding lattice extends to infinity and is periodic.
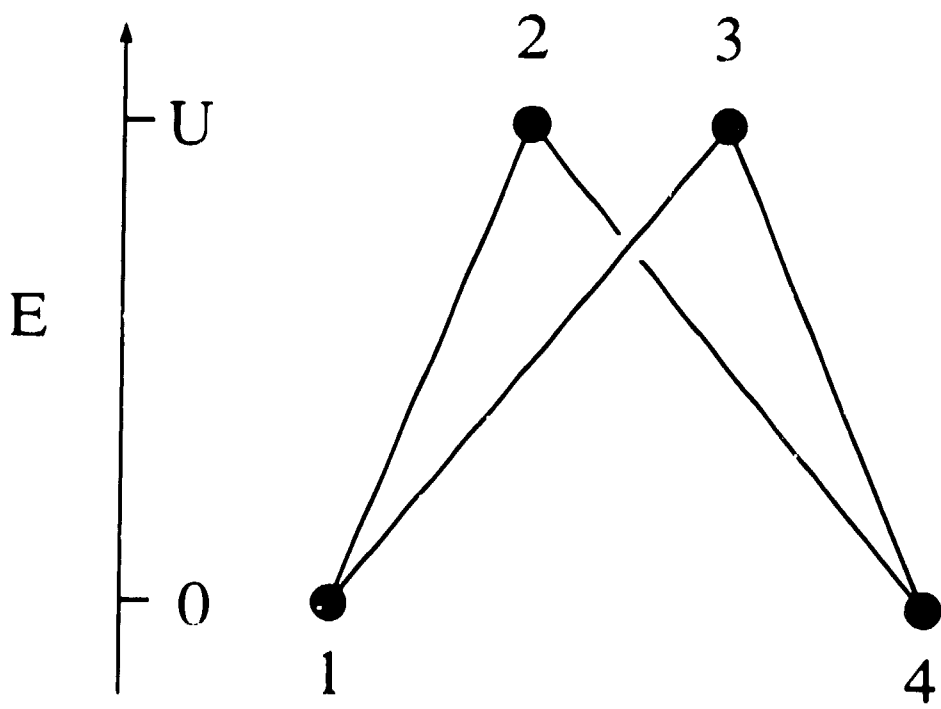
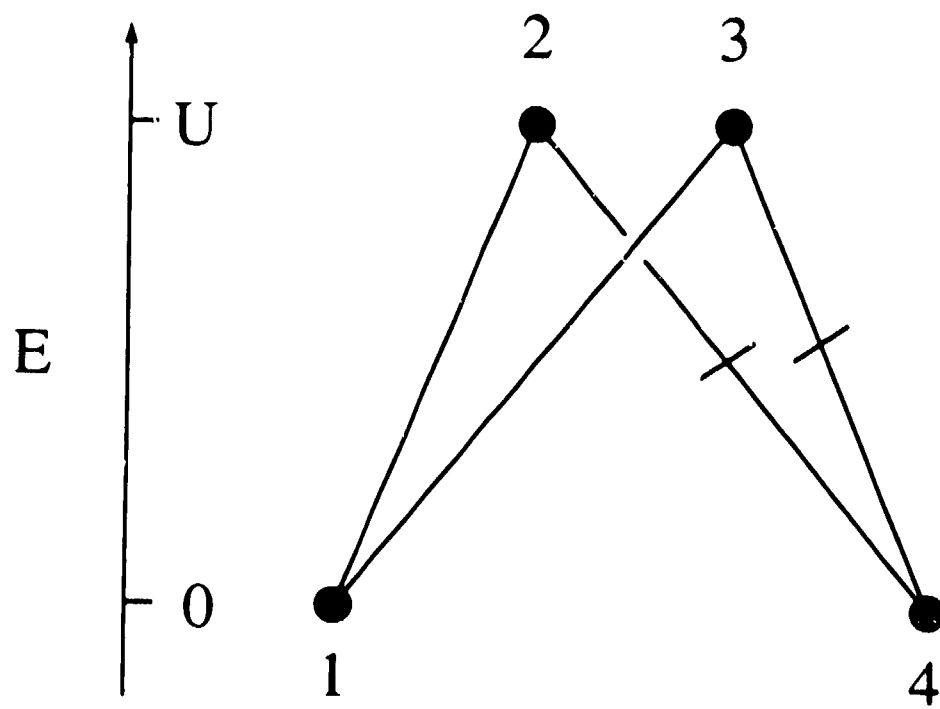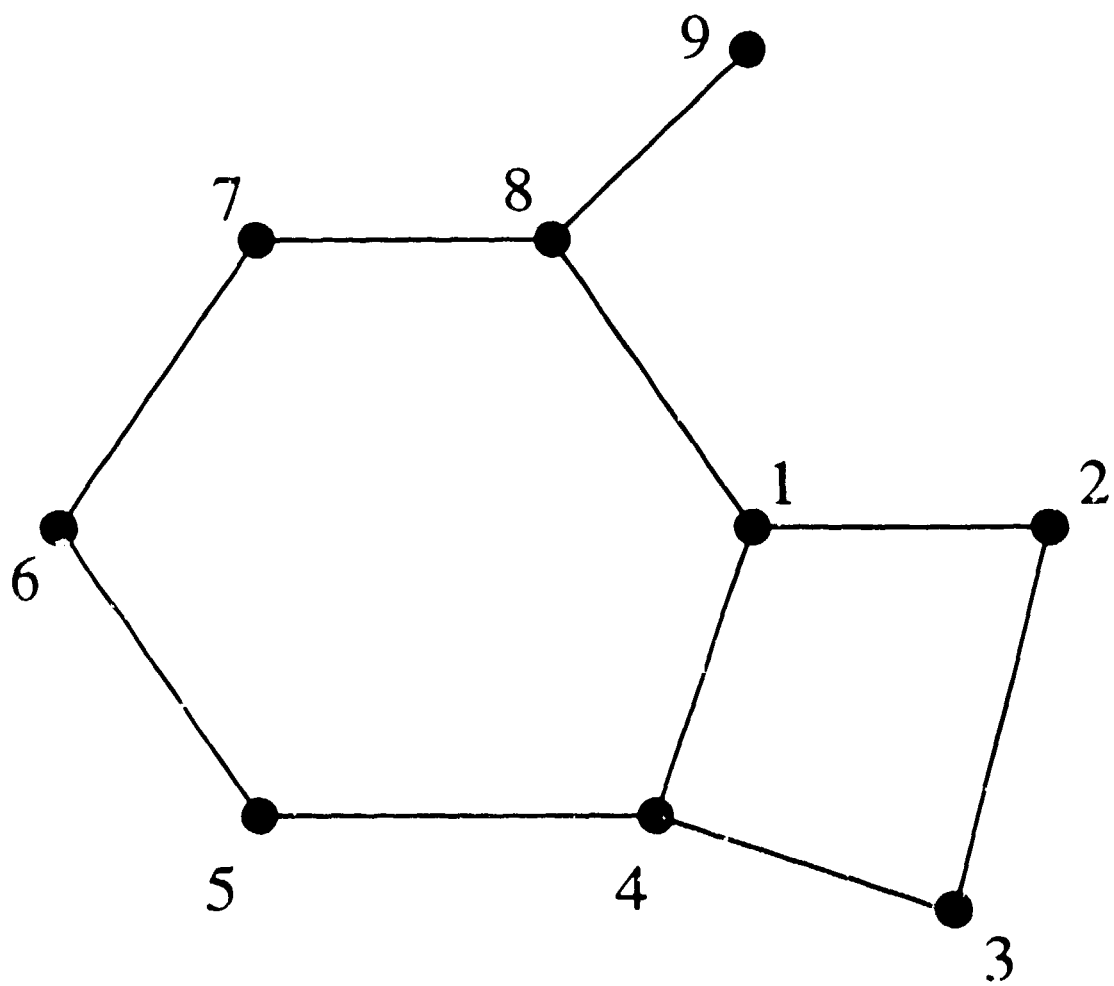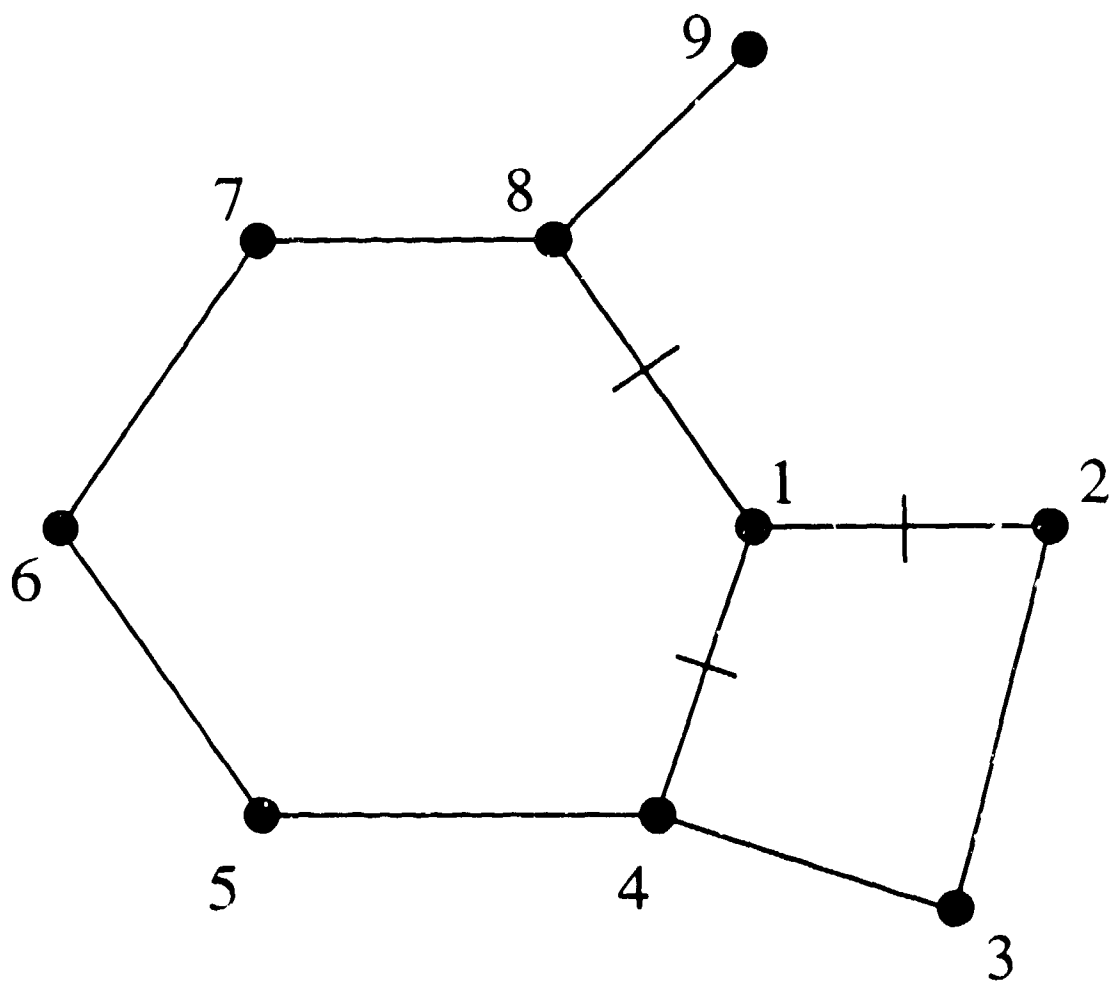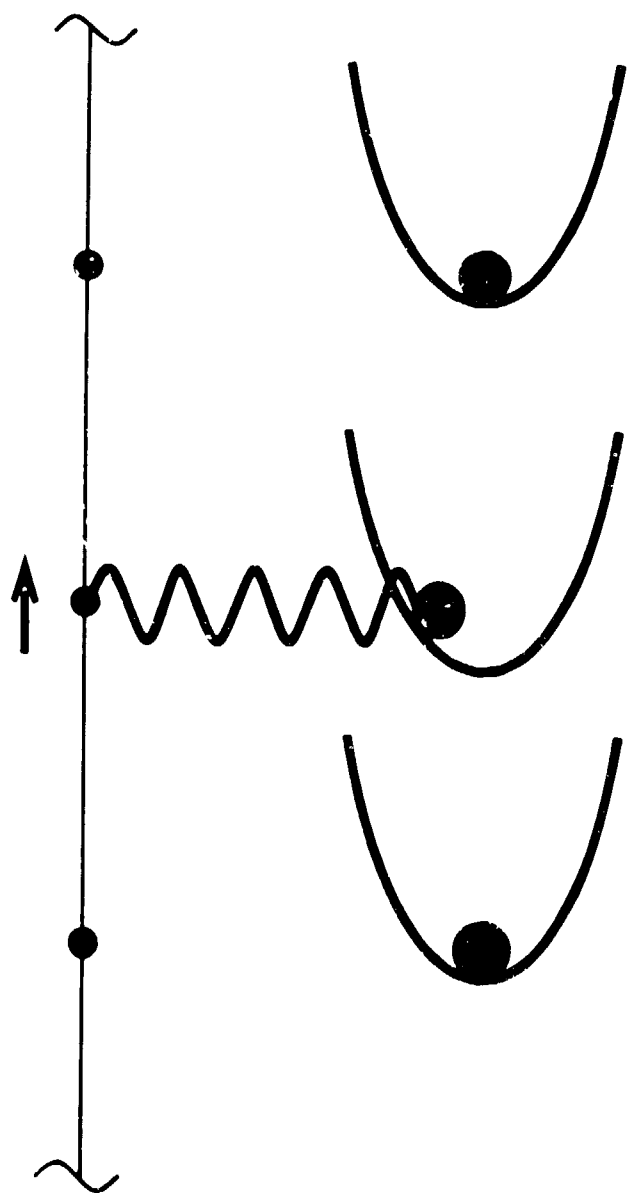**Figure 12**   The eigenvalues of the polaron problem is plotted as a function of wavevector k.
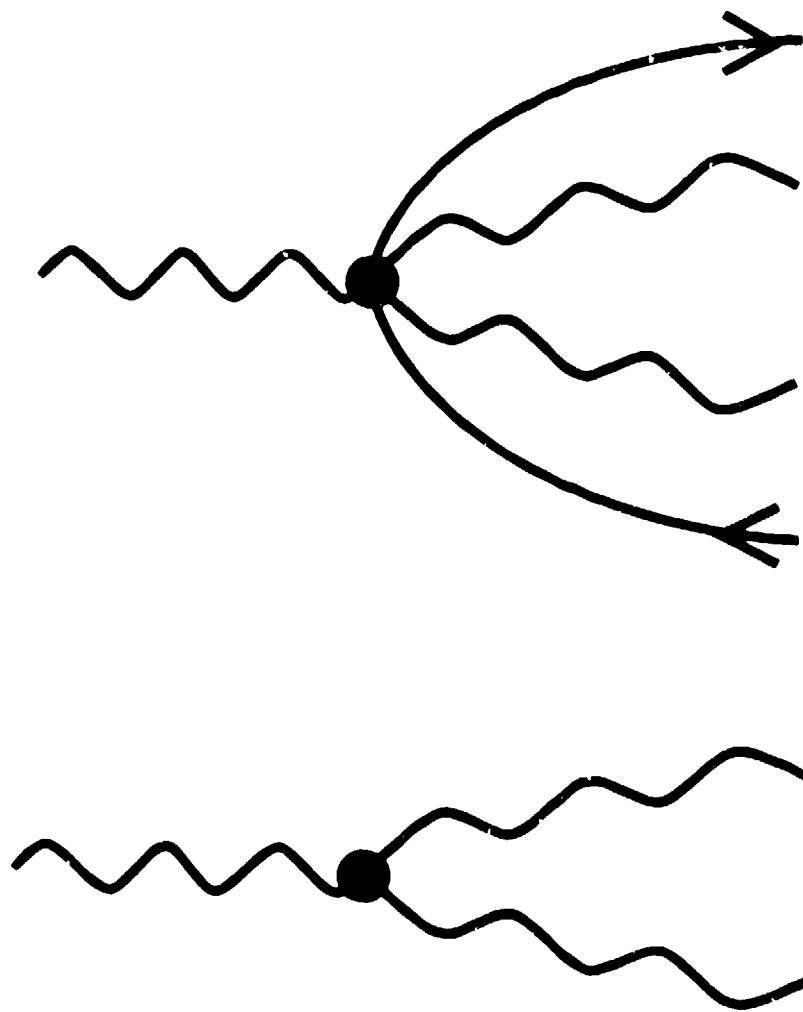
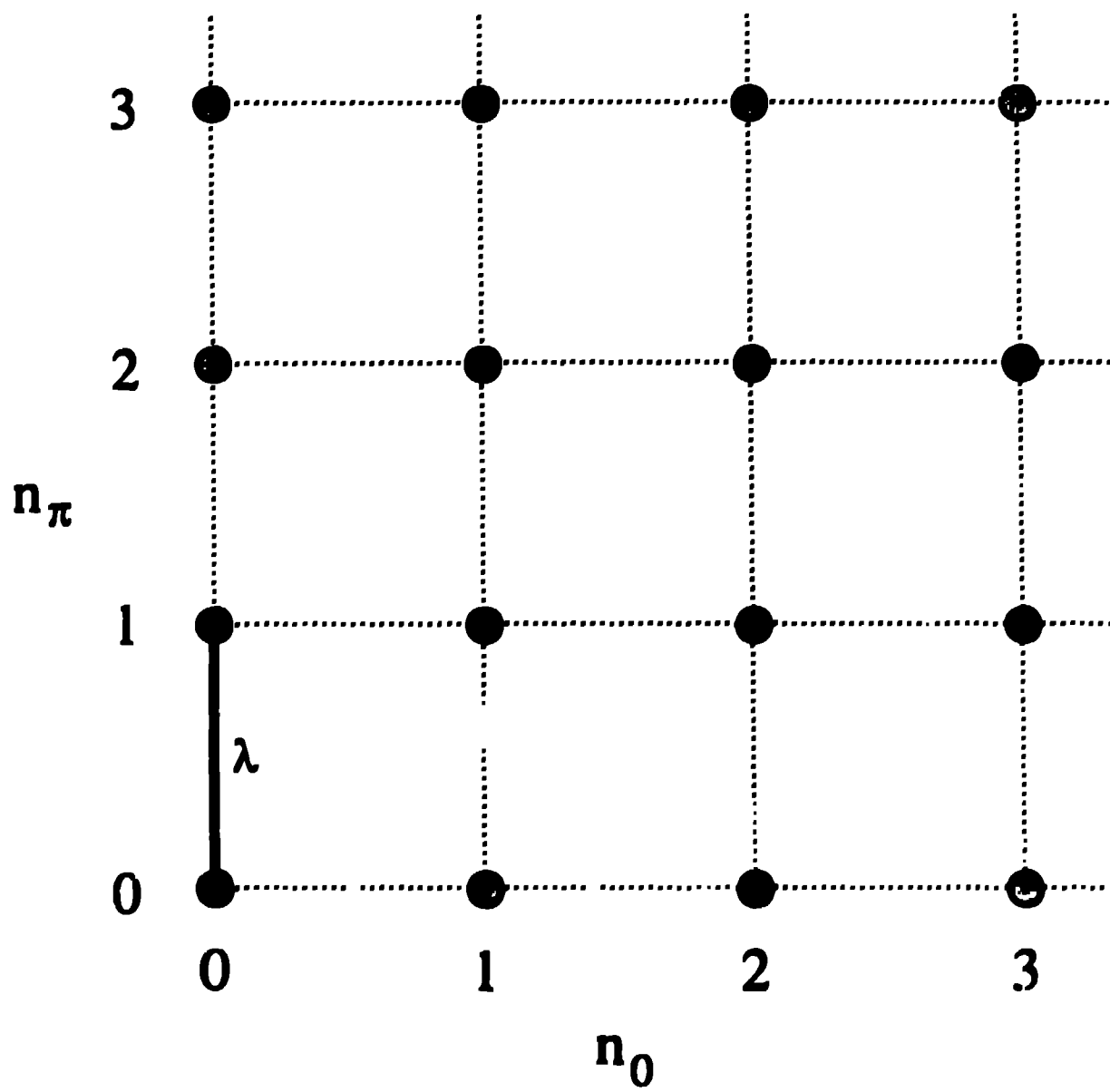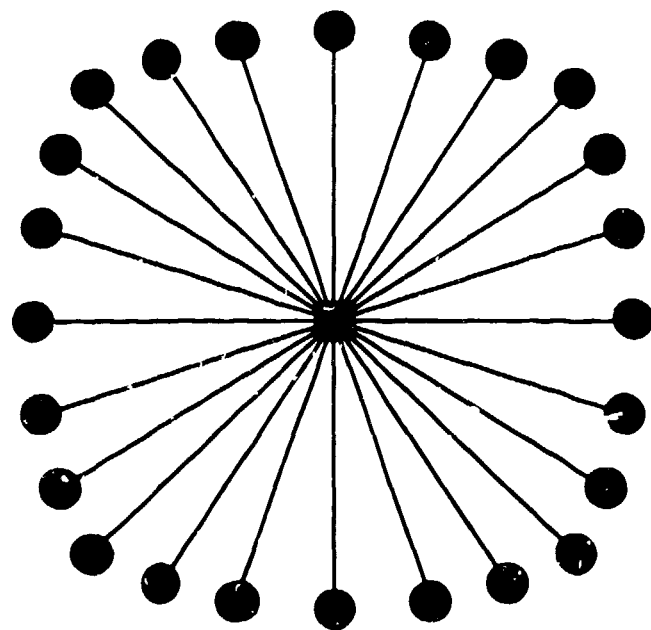Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5
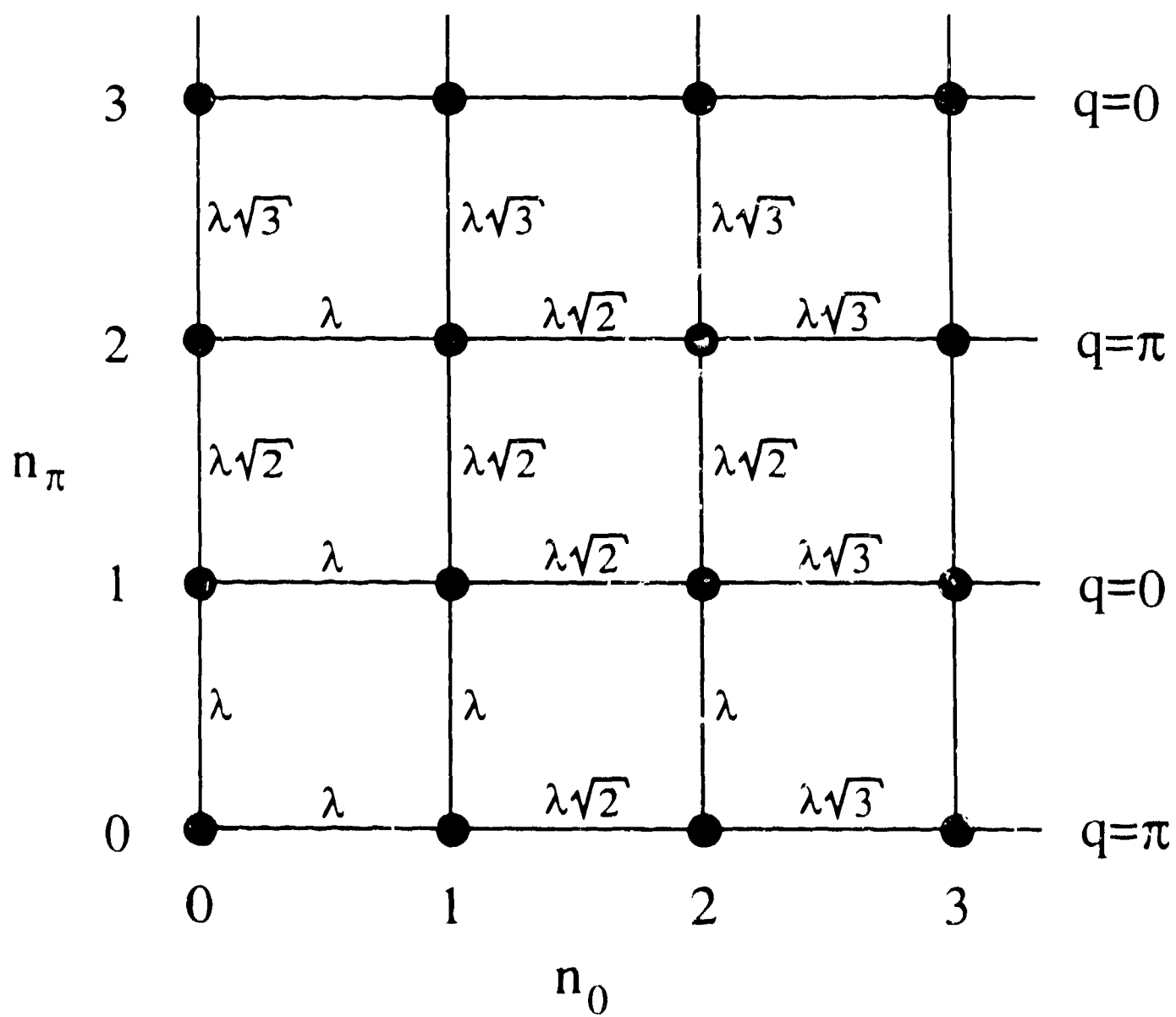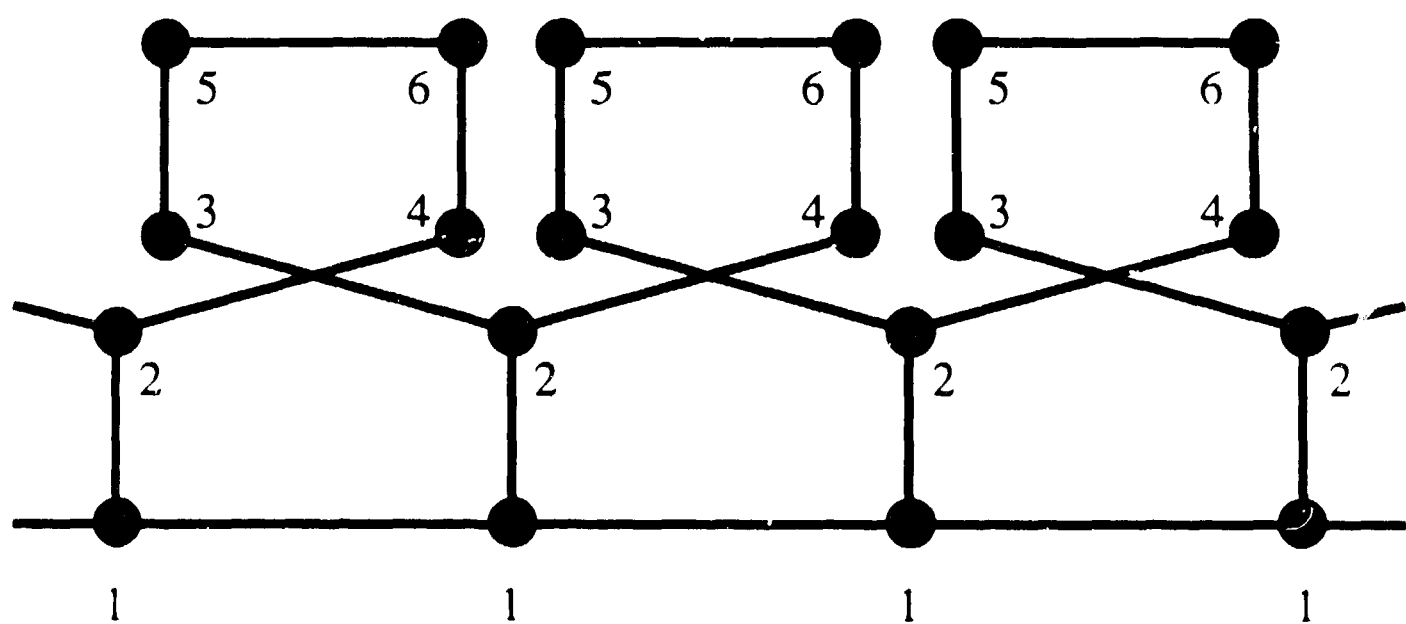
Fig. 6
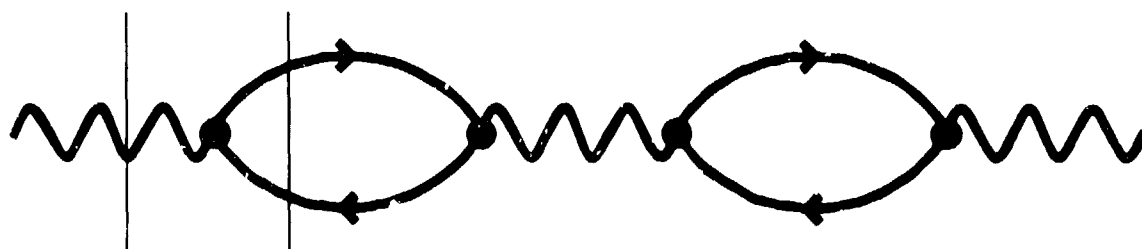
Fig. 7

Fig. 8

Fig. 9

(a)

(b)
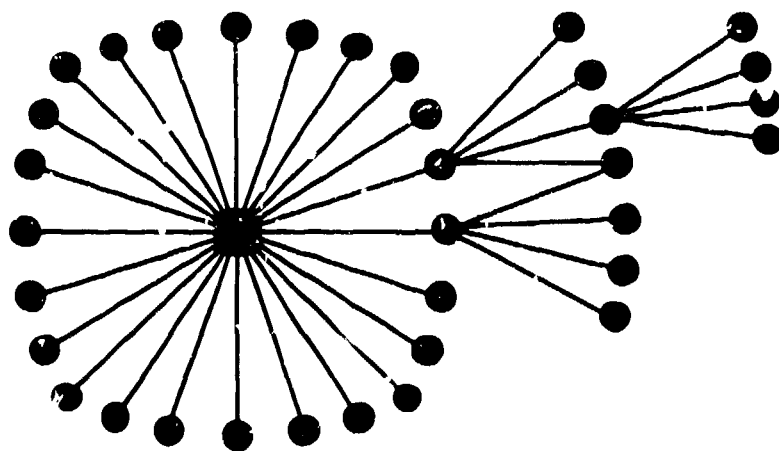
Fig. 10

Fig. 11

t and Lambda= 1.00 1.00
no. of phonons =3
nup =1
ndown =0
no. of states=100

Fig 12